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Zinc mercury(II) tetrakis(selenocyanate)

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.007 Å; R factor = 0.026; wR factor = 0.053; data-to-parameter ratio = 37.7.

The title crystal, $[HgZn(NCSe)_4]_n$, a coordination polymer, has a diamond-like network. In the crystal, the metal ions, Zn^{2+} and Hg^{2+}, are both located on fourfold inversion axes and mimic the role of C atoms in the structure of diamond, and the linear selenocyanate bridges replace the C—C bonds. The C—N—Zn unit is almost linear and the C—Se—Hg unit is nearly a right angle. Thus, the $HgZn_4$ (or $ZnHg_4$) arrangement is midway between a tetrahedron and a square plane, with two types of Hg—Zn—Hg (or Zn—Hg—Zn) angles of 92.38 (6) and 156.45 (6)°.

Related literature

For background to coordination polymers, see: Batten *et al.* (2009). For diamond-like networks, see: Sun *et al.* (2006); Evans *et al.* (1999). For similar structures, see: Wang *et al.* (2001, 2007); Sun *et al.* (2005, 2006); Tian *et al.* (1999); Xu *et al.* (1999); Yan *et al.* (1999); Yuan *et al.* (1997).

Experimental

Crystal data

$[HgZn(NCSe)_4]$
M_r = 685.88
Tetragonal, $I\bar{4}$
a = 11.2716 (1) Å
c = 4.6981 (1) Å
V = 596.89 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 27.02 mm^{-1}
T = 293 K
0.13 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.127, T_{max} = 0.173
2476 measured reflections
1244 independent reflections
1113 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.053
S = 0.86
1244 reflections
33 parameters
$\Delta\rho_{max}$ = 1.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}
Absolute structure: Flack (1983), 467 Friedel pairs
Absolute structure parameter: 0.026 (10)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2230).

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supplementary materials

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Zinc mercury(II) tetrakis(selenocyanate)

Hai-Qing Sun, Xin-Qiang Wang and Wei-Wei Zhang

1. Comment

Coordination polymers, which contain ions linked by coordinated ligands into an infinite array, have extensive applications such as porosity, magnetism, non-linear optical activity, reactive networks, heterogenous catalysis and luminescence (Batten *et al.* 2009). $[AB(SCN)_4]_n$ and $[AB(SeCN)_4]_n$ (where A and B = Zn, Cd, Hg or Mn) are coordination polymers that have non-linear optical property (Wang *et al.*, 2007, 2001; Sun *et al.*, 2006, 2005; Yuan *et al.* 1997). $[ZnHg(SeCN)_4]_n$ is a new member of this group.

All the $[AB(SCN)_4]_n$ and $[AB(SeCN)_4]_n$ have similar structure. The $[ZnHg(SeCN)_4]_n$ is of no exception. The Zn and Hg atoms are connected by $SeCN^-$ ions, forming an infinite three-dimensional network (see Fig. 1). Each Zn or Hg node is 4-coordinated with Zn—N or Hg—Se bond. The ZnN_4 and $HgSe_4$ tetrahedra are slightly distorted from an ideal one. The Zn—N—C—Se is nearly linear, but the C—Se—Hg is bent. The whole structure might be defined as a diamond-like network with Zn and Hg nodes and bent bonds. The $HgZn_4$ (or $ZnHg_4$) tetrahedra have a significant distortion from an ideal one, with two types of Hg—Zn—Hg (or Zn—Hg—Zn) angles, 92.38 (6)° and 156.45 (6)°. Along the c-direction there are irregular octagon channels.

2. Experimental

Sodium metasilicate nonahydrate ($Na_2SiO_3.9H_2O$), $ZnCl_2$ and KSeCN solution were mixed together with stirring for 1 h. Then the sol is put into a test tube. Glacial acetic acid was added to adjust pH to 3.1. The above solution was sealed and gelled on standing for 72 h. Then some $HgCl_2$ solution was added on top of the gel. Within 20 d the ZMSC crystal grew in the gel medium.

3. Refinement

The unusually large residual electron density (1.347 e Å^{-3}) is found near the Hg atoms.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

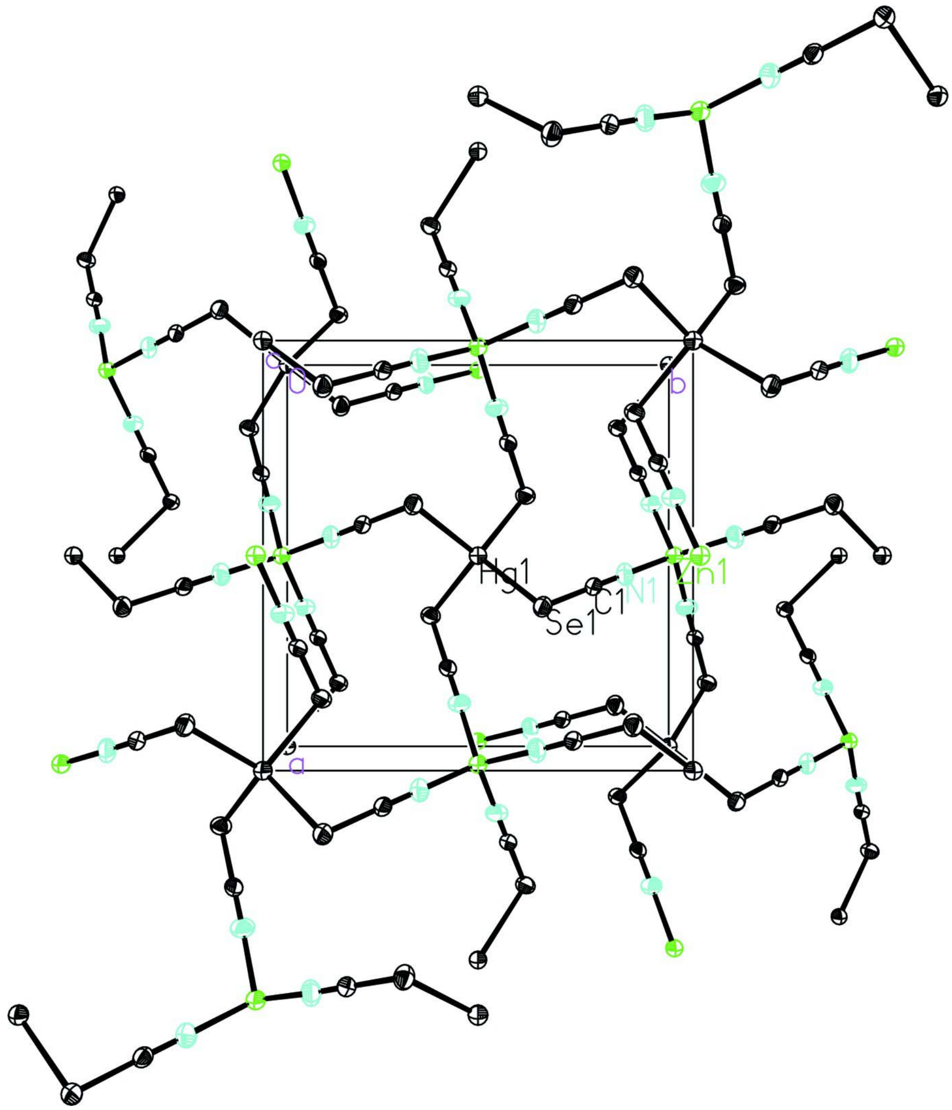

Figure 1

Packing diagram of $[ZnHg(NCSe)_4]_n$ (viewed down the *c* axis), with displacement ellipsoids drawn at the 50% probability level.

Zinc mercury(II) tetrakis(selenocyanate)

Crystal data

$[HgZn(NCSe)_4]$	D_x = 3.816 Mg m^{-3}
M_r = 685.88	Mo $K\alpha$ radiation, λ = 0.71073 Å
Tetragonal, $I\bar{4}$	Cell parameters from 1556 reflections
Hall symbol: I -4	θ = 2.6–34.8°
a = 11.2716 (1) Å	μ = 27.02 mm^{-1}
c = 4.6981 (1) Å	T = 293 K
V = 596.89 (2) Å^3	Prism, colourless
Z = 2	0.13 × 0.12 × 0.10 mm
F(000) = 596	

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.127, T_{max} = 0.173
2476 measured reflections
1244 independent reflections
1113 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 38.1°, θ_{min} = 2.6°
$h = -16 \rightarrow 19$
$k = -17 \rightarrow 11$
$l = -6 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.053
S = 0.86
1244 reflections
33 parameters
0 restraints
Primary atom site location: isomorphous structure methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0047 (3)
Absolute structure: Flack (1983), 467 Friedel pairs
Absolute structure parameter: 0.026 (10)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Hg1	0.0000	0.0000	0.0000	0.02909 (11)
Se1	0.12160 (4)	0.15390 (4)	0.31572 (11)	0.03115 (13)
Zn1	0.0000	0.5000	−0.2500	0.0289 (2)
N1	0.0462 (4)	0.3643 (3)	−0.0118 (16)	0.0374 (9)
C1	0.0756 (4)	0.2818 (4)	0.1106 (10)	0.0280 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.02405 (11)	0.02405 (11)	0.0392 (2)	0.000	0.000	0.000
Se1	0.0322 (2)	0.0250 (2)	0.0363 (3)	−0.00208 (18)	−0.0073 (2)	0.00031 (19)
Zn1	0.0242 (3)	0.0242 (3)	0.0382 (6)	0.000	0.000	0.000
N1	0.040 (2)	0.0242 (16)	0.048 (2)	0.0011 (14)	−0.004 (3)	−0.004 (2)
C1	0.0241 (19)	0.0219 (18)	0.038 (2)	−0.0019 (15)	0.0023 (17)	−0.0046 (17)

Geometric parameters (Å, º)

Hg1—Se1	2.6623 (5)	Zn1—N1^{iv}	1.966 (6)
Hg1—Se1^{i}	2.6623 (5)	Zn1—N1^{v}	1.966 (6)
Hg1—Se1^{ii}	2.6623 (5)	Zn1—N1^{vi}	1.966 (6)
Hg1—Se1^{iii}	2.6623 (5)	Zn1—N1	1.966 (6)
Se1—C1	1.810 (5)	N1—C1	1.141 (7)
Se1—Hg1—Se1^{i}	108.084 (11)	N1^{iv}—Zn1—N1^{vi}	110.6 (4)
Se1—Hg1—Se1^{ii}	112.28 (2)	N1^{v}—Zn1—N1^{vi}	108.91 (18)
Se1^{i}—Hg1—Se1^{ii}	108.084 (11)	N1^{iv}—Zn1—N1	108.91 (18)
Se1—Hg1—Se1^{iii}	108.084 (11)	N1^{v}—Zn1—N1	110.6 (4)
Se1^{i}—Hg1—Se1^{iii}	112.28 (2)	N1^{vi}—Zn1—N1	108.91 (18)
Se1^{ii}—Hg1—Se1^{iii}	108.084 (11)	C1—N1—Zn1	175.5 (6)
C1—Se1—Hg1	94.29 (14)	N1—C1—Se1	178.1 (5)
N1^{iv}—Zn1—N1^{v}	108.91 (18)		
Se1^{i}—Hg1—Se1—C1	−14.76 (14)	N1^{iv}—Zn1—N1—C1	69 (5)
Se1^{ii}—Hg1—Se1—C1	−133.89 (14)	N1^{vi}—Zn1—N1—C1	−52 (5)
Se1^{iii}—Hg1—Se1—C1	106.99 (14)	Hg1—Se1—C1—N1	140 (12)

Symmetry codes: (i) $-y, x, -z$; (ii) $-x, -y, z$; (iii) $y, -x, -z$; (iv) $y-1/2, -x+1/2, -z-1/2$; (v) $-x, -y+1, z$; (vi) $-y+1/2, x+1/2, -z-1/2$.